



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 09:42 am BST

PDB ID : 1MIO
Title : X-RAY CRYSTAL STRUCTURE OF THE NITROGENASE
MOLYBDENUM-IRON PROTEIN FROM CLOSTRIDIUM PASTEURIANUM AT 3.0 ANGSTROMS RESOLUTION
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Deposited on : 1993-03-24
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

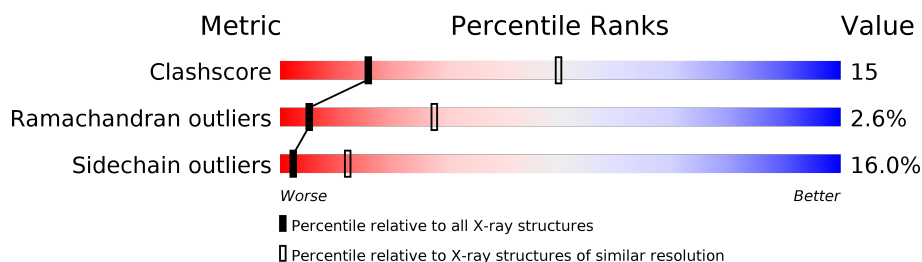
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	
1	C	533	
2	B	458	
2	D	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	B	496	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	D	496	-	-	X	-
6	CLP	B	498	-	-	X	-
6	CLP	D	498	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4074	2588	682	777	27			
1	C	525	Total	C	N	O	S	0	0	0
			4077	2589	683	778	27			

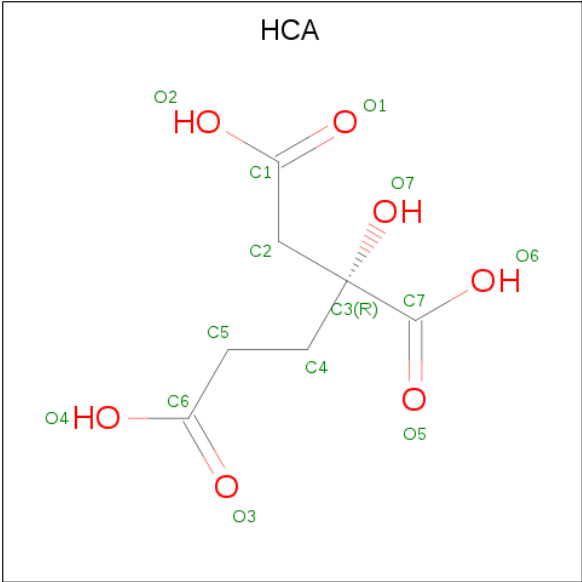
- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			
2	D	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

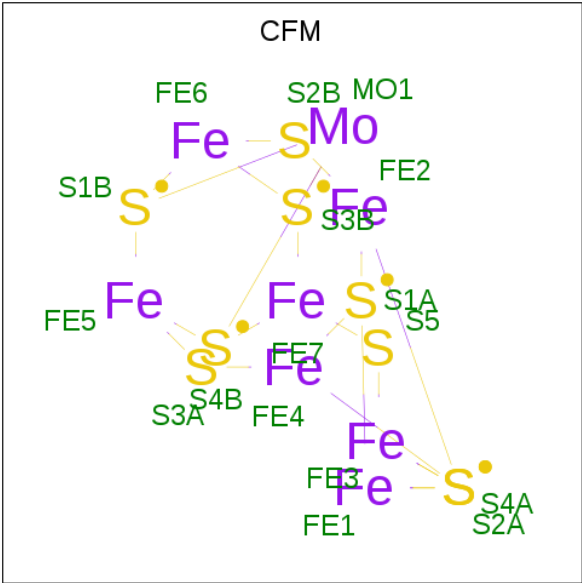
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



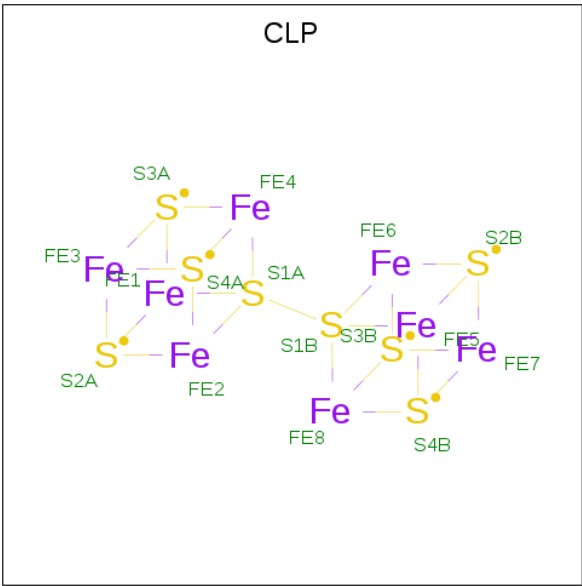
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			14	7	7		
4	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe₇MoS₉).

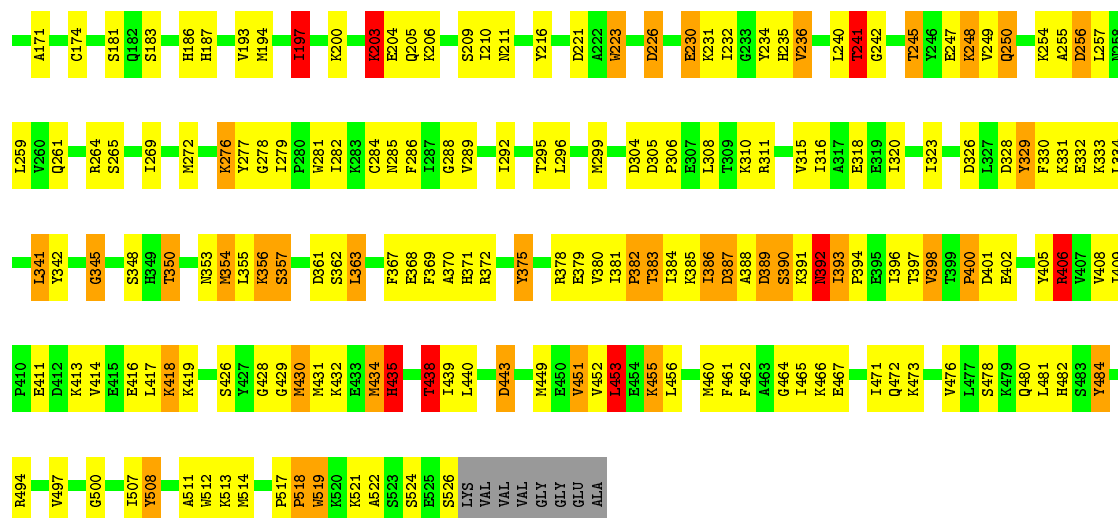


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	D	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE-S CLUSTER (three-letter code: CLP) (formula: Fe₈S₈).

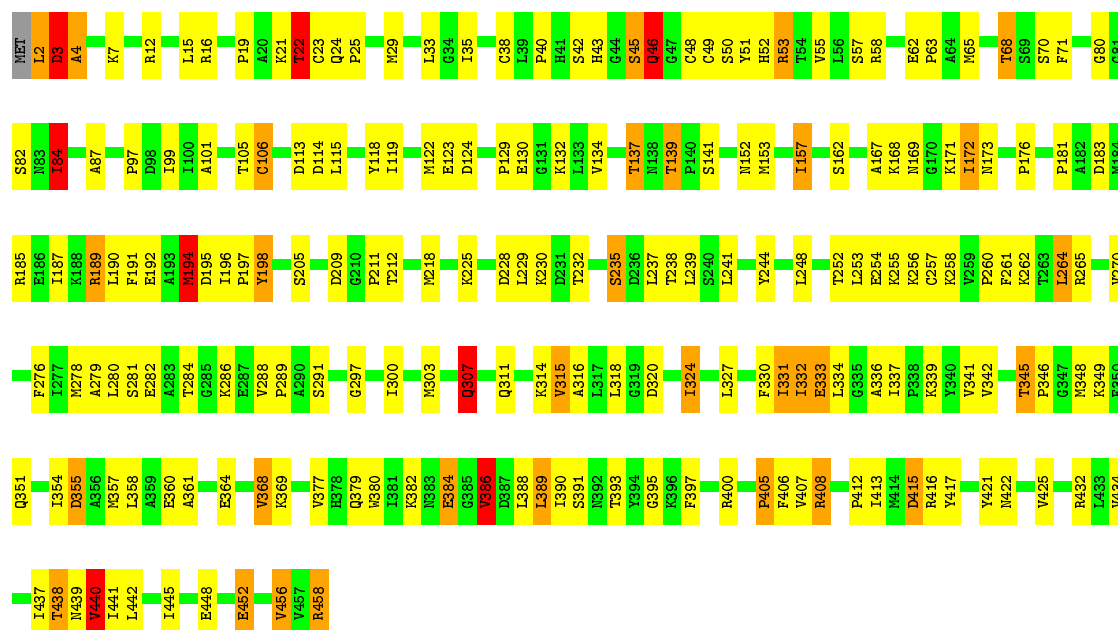


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			16	8	8		
6	D	1	Total	Fe	S	0	0
			16	8	8		



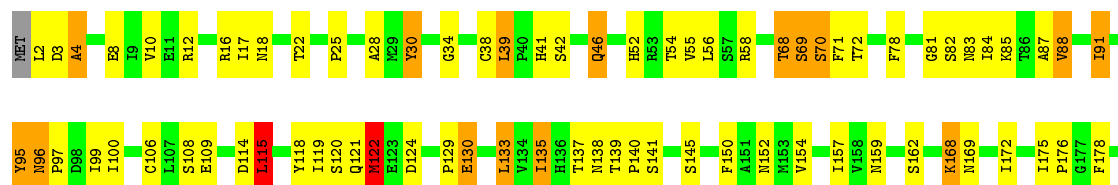
• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain B: 56% 35% 7%



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain D: 57% 33% 8%



P181	T263	S366	V457
M184	L264	K367	R458
R185	R265	V368	
K188	V270	D373	
R189	I277	D376	
L190	M278	V377	
F191	K286	W380	
E192	E287	E384	
M194	S291	G385	
D195	I292	V386	
Y198	E293	D387	
F201	R296	L388	
P202	D301	L389	
D203	I304	I390	
T204	I304	S391	
V207	Q307	R392	
L208	Q308	T393	
P211	Q311	Y394	
Y216	V315	G395	
K217	A316	K396	
M218	L317	A399	
Y219	L318	R400	
P220	G319	E401	
E221	D320	E402	
T224	P321	N403	
L229	I325	I404	
G233	A326	P405	
N234	L327	F406	
S235	S328	V407	
L239	K329	R416	
S240	E333	Y420	
S246	K339	Y427	
D247	Y340	K428	
L248	V341	I431	
G249	V342	E436	
A250	T343	I437	
L253	G344	T438	
E254	T345	N439	
K255	P346	V440	
R256	F350	R447	
C257	Q351	E448	
K258	I354	C449	
V259	D355	T450	
P260	A356	E451	
F261	M357	E452	
K262	L358	D453	
		V456	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.96 Å 151.30 Å 121.90 Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CFM, CLP, HCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	0/4163	1.90	105/5629 (1.9%)
1	C	0.98	3/4166 (0.1%)	1.84	95/5631 (1.7%)
2	B	0.91	0/3582	1.75	65/4845 (1.3%)
2	D	0.93	3/3582 (0.1%)	1.78	69/4845 (1.4%)
All	All	0.94	6/15493 (0.0%)	1.82	334/20950 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	5
2	B	0	2
2	D	0	4
All	All	0	13

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	141	SER	CA-CB	-6.37	1.43	1.52
1	C	390	SER	CA-CB	5.89	1.61	1.52
1	C	451	VAL	CA-CB	5.82	1.67	1.54
1	C	197	ILE	CA-CB	5.75	1.68	1.54
2	D	130	GLU	CB-CG	5.40	1.62	1.52

The worst 5 of 334 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	A	240	LEU	CA-C-N	-12.72	89.21	117.20
1	A	390	SER	N-CA-C	11.99	143.38	111.00
1	A	240	LEU	O-C-N	11.33	140.83	122.70
1	C	406	ARG	NE-CZ-NH1	10.82	125.71	120.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	240	LEU	Mainchain
2	B	198	TYR	Sidechain
2	B	337	ILE	Peptide
1	C	32	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	3992	137	0
1	C	4077	0	3999	149	0
2	B	3511	0	3495	96	0
2	D	3511	0	3495	91	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	14	0	6	0	0
4	D	14	0	6	2	0
5	B	17	0	0	4	0
5	D	17	0	0	4	0
6	B	16	0	0	4	0
6	D	16	0	0	5	0
All	All	15269	0	14993	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 444 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:498:CLP:S1A	6:B:498:CLP:S1B	2.30	1.28
6:D:498:CLP:S1B	6:D:498:CLP:S1A	2.33	1.26
1:C:345:GLY:HA3	5:D:496:CFM:S1A	2.01	0.99
1:C:197:ILE:HD11	1:C:249:VAL:HB	1.43	0.99
2:D:162:SER:HB3	2:D:257:CYS:SG	2.06	0.96

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/533 (98%)	447 (86%)	58 (11%)	18 (3%)	3	20
1	C	523/533 (98%)	452 (86%)	51 (10%)	20 (4%)	3	18
2	B	455/458 (99%)	414 (91%)	35 (8%)	6 (1%)	12	45
2	D	455/458 (99%)	411 (90%)	37 (8%)	7 (2%)	10	42
All	All	1956/1982 (99%)	1724 (88%)	181 (9%)	51 (3%)	5	27

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	143	ALA
1	A	241	THR
1	A	387	ASP
1	A	411	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/446 (97%)	355 (82%)	79 (18%)	1	9
1	C	435/446 (98%)	369 (85%)	66 (15%)	3	14
2	B	383/384 (100%)	322 (84%)	61 (16%)	2	12
2	D	383/384 (100%)	327 (85%)	56 (15%)	3	15
All	All	1635/1660 (98%)	1373 (84%)	262 (16%)	2	12

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	332	ILE
1	C	41	THR
2	D	311	GLN
2	B	360	GLU
2	B	437	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
1	C	237	ASN
2	D	308	GLN
2	B	439	ASN
1	C	261	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HCA	B	494	-	4,13,13	0.81	0	4,18,18	2.47	3 (75%)
4	HCA	D	494	-	4,13,13	0.75	0	4,18,18	2.88	3 (75%)
5	CFM	D	496	1	0,24,24	0.00	-	-		
6	CLP	B	498	1,2	0,25,25	0.00	-	-		
6	CLP	D	498	1,2	0,25,25	0.00	-	-		
5	CFM	B	496	1	0,24,24	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	B	494	-	-	7/7/17/17	-
4	HCA	D	494	-	-	4/7/17/17	-
6	CLP	D	498	1,2	-	-	0/12/10/10
6	CLP	B	498	1,2	-	-	0/12/10/10

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	494	HCA	C4-C5-C6	4.47	118.16	111.39
4	B	494	HCA	C4-C5-C6	3.91	117.32	111.39
4	D	494	HCA	C4-C3-C7	-2.50	107.12	111.52
4	D	494	HCA	C3-C2-C1	2.45	118.90	114.98
4	B	494	HCA	C4-C3-C7	2.10	115.23	111.52

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	494	HCA	C1-C2-C3-C4
4	B	494	HCA	C1-C2-C3-C7
4	B	494	HCA	C1-C2-C3-O7
4	B	494	HCA	C2-C3-C4-C5
4	B	494	HCA	C7-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	494	HCA	2	0
5	D	496	CFM	4	0
6	B	498	CLP	4	0
6	D	498	CLP	5	0
5	B	496	CFM	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.